

Mike.Teague@clariant.com 11/16/2006 04:51 PM

- To Kimberly Tisa/R1/USEPA/US@EPA, Laura Casey/DC/USEPA/US@EPA
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bcc

Subject Calculation Guidance Document and Spreadsheets

Kim -

Here are the files that Versar requested. There are two spreadsheets (one is zipped in hopes of reducing any problems with email), and a calculations guide document which is a step-by-step explanation for how the equations were developed and used in the spreadsheets.

The recent delay was caused by questions that Clariant had regarding some differences between acceptable carpet concentrations as presented in Table 2 of the August 18, 2006 addendum and Table 4 of the attached calculations guide. As BBL notes in the guide, the acceptable concentration values for RF=1 changed substantially due to the modification of exposure durations for this factor, as well as incorporation of EPA-required room air exchange rate values. Acceptable concentration values for RF's other than 1 did not change significantly; therefore, the ultimate conclusion is the same as that presented by the August 18, 2006 submittal.

If, after reviewing these files, EPA and Versar still have questions regarding how the acceptable values were calculated, Clariant recommends that Versar and BBL be allowed to speak directly with each other, in the presence of EPA and Clariant, to reach an acceptable resolution.

Best regards,

Mike

This E-Mail message contained an attachment which is a computer program. This attached computer program could contain a computer virus which could cause harm to EPA's computers, network, and data. The attachment has been deleted.

This was done to limit the distribution of computer viruses introduced into the EPA network. We are deleting all computer program attachments sent from the Internet into the agency via E-Mail.

If the message sender is known and the attachment was legitimate, you should contact the sender and request that they rename the file name extension and resend the E-Mail with the renamed attachment. After receiving the revised E-Mail, containing the renamed attachment, you can rename the file extension to its correct name.

For further information, please contact the EPA Call Center at



(866) 411-4EPA (4372). The TDD number is (866) 489-4900.
******************* ATTACHMENT NOT DELIVERED ****************
[Attachment PCB Air Concentration Decay_FOR_EPA_2AP.zip removed]
EXPOSURE MODEL_CLARIANT_FIBER_SCENARIO INVERSE FOR EPA 2AP.xls CALCULATIONS GUIDE FOR EPA 2AP.x

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INVERSE NON-CANCER Inputs:	THQ=Target hazard quotient RtD=Reference dose (mg/kg bw/day) (USEPA, 1996) AT=Averaging time (days) (ED*365)	ED=Exposure duration (yrs) EF=Exposure frequency (days/yr) Carpet life expectancy 7- 10 years	IR=Dust (soit) ingestion rate (mg/day) AF≖Dust adherence factor for children post-activity indoors on hands, arms, legs, feet (mg/dn	SA=Contact skin surface area during warm-weather play with 32% skin exposed (¿dday) BW-Ebody weight (children 6 mrihis to 12 yrs old; kg) BRoAF≡Chrai biosvallablity factor frimitses t	UR-inhatation rate (rikgay) VP≠Vator ressure of PCA4470 m/vivor ras	d"=Carpet (hickness (m)	M=Campels area mass (face weight; mg/m²) A==Compels com air exchange rate (1/week; based on recommended 0.35 exchanges/hr)	יברית במונים או מונים או מונים DERM בשרותים עומים או מונים א Employer (מונים או מונים או מ	(SSARIER) (GRADER)	Dermai C = (THQ x BW x AT) / ED x EF [(1//RID x SA x AF x 1/1000000 x DERM)] C=Acceptable concentration in carpet fiber (mg/kg)	DERM 0.14 5682.4

Ingestion $C = (THQ \times BW \times AT) / ED \times EF \{ (1/R1D \times IR \times 1/1000000 \times BioAF) \} \\ C = Acceptable concentration in carpet fiber (mg/kg)$ Ingestion Alone 28934.5 5786.9 2893.5 576.7 289.3 5682.4 BloAF 0.0† 0.05 0.1 0.5

Inhalation - Volatife Based on Empirical Data, Vapor Pressure, and Mass Balance Models

Surface-air paniton coefficient for carpet (unitless) $- \text{Kca} = (M_d) / \text{dw} = 10^{3.22.0.826q vP}$

144515.211807 Bennet and Furlaw (2004) EST38: 2142-2152

M (mg/m2)=C_x*d_x*10^{3 82 62 bayre} M/C_x = d_x*10^{3 82 62 bayre</sub> C_{csyo} (mg/kg) = M (mg/m2)Wass (kg/m2) VF (m3/kg)=[d_x (m)*10^{4 82 63 bayre}][Mass_(mg/m2)/1000000 (mg/kg)]/AE} 0.01 9817.4

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0.005 Inhalation Alone 0.001 98173.6 Ҡ

ingestion, Demail, and inhalation Combined $G = \{THQ \times BW \times T \} = TW \times T \} = TW \times T = TW \times T$

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I Albert 14 China Control Control	0.01 3201.0 2219.0 1604.0 498.5 267.8
	0.005 3824.5 2801.8 1746.7 511.5 271.5
	0.001 4530,4 2785,7 1880,5 522.4 274,6
	All Combined 0.0001 4726.8 2858.7 1913.5 524.9 275.2
	BioAF/RF 0.01 0.05 0.1 0.5

Read results for a given AF/RE/ED/EF combination in this table



NVERSE CANCER

Inputs:

⁻R≕Target cancer risk

SF=Cancer slope factor

ATD=Acceptable cancer dose (mg/kg bw/d)

AT_c=Averaging time for carcinogens (days)

ED_L=Exposure duration (carpet life; yrs)

EF=Exposure frequency (days/yr)

Carpet life expectancy 7- 10 years

IR=Dust (soil) ingestion rate (mg/day)

AF≍Soil adherence factor for children post-activity indoors on hands, arms, legs, feet (mg/cm²)

SA=Contact skin surface area during warm-weather play with 32% skin exposed (cm²/day)

BW=Body weight (children 6 mnths to 12 yrs old; kg)

BioAF=Bioavailablity factor (unitless)

IHR-inhalation rate (m³/day)

VP=Vapor pressure of PCB44/70 mixture (Pa)

d_w=Carpet thickness (m)

Carpet mass=Carpet area mass (face weight; kg/m²)

AE=Complete room air exchange rate (1/week; based on recommended 0.35 exchanges/hr) C_g=Air concentration in an enclosed space after 7 days post-installation (mg/m³)

DERM= Dermal uptake factor (US EPA)

RF=Retention factor (unitless)

Dermai

 $C = (BW \times AT_c) / ED_L \times EF [(1/ATD \times SA \times AF \times 1/1000000 \times DERM)]$

C=Acceptable concentration in carpet fiber (mg/kg)

Dermal Alone

M 0.14 284120.0



Ingestion

 $C = (BW \times AT_c) / ED_L \times EF [(1/ATD \times IR \times 1/1000000 \times BioAF)]$ C=Acceptable concentration in carpet fiber (mg/kg)

Ingestion Alone 289345.5 144672.7 1446727.3 28934.5 14467.3 0.05 BioAF

Inhalation - Volatile

Based on Empirical Data, Vapor Pressure, and Mass Balance Models

Surface-air parition coefficient for carpet (unitless) $Kca=(k_s/k_d)/dw=10^{3.82-0.62logVP}$

 $M (mg/m2) = C_{air}^* d_w^* 10^{3.83-0.62logVP}$ $k_s/k_{d} = M/C_{air} = d_w^{\ *} + 0^{3.83 - 0.62 iogVP}$

 $M/C_{air} = d_w^* 10^{3.83-0.62 log VP}$

 C_{carpet} (mg/kg) = M (mg/m2)/Mass_c (kg/m2)

VF (m3/kg)=[d_w(m)*10^{3.83-0.62logVP}]/[Mass_c(mg/m2)/1000000 (mg/kg)]/AE

Inhalation Alone

981735.7 0.005 0.0 0.001 4908678.4 몺

490867.8 0.0

0.01

0.07636

Ingestion, Dermal, and Inhalation Combined

 $C = (BW \times AT_c) / ED_L \times EF [(1/ATD \times IR \times 1/1000000 \times BioAF) + (1/ATD \times SA \times AF \times 1/1000000 \times DERM) + (1/ATD \times IHR N) + (1/ATD N) + (1/ATD N) + (1/ATD N)$

0.001 All Combined

0.0001

0.005



191224.4	125088.8	87333.2	25576.1	13575.9
226522.4	139286.7	94024.6	26120.5	13727.8
236338.1	142937.0	95674.0	26246.2	13762.4
0.01	0.05	0.1	0.5	•

Read results for a particular AF/RE/ED/EF combination in this table



1.00E-06 0.07 0.00001429 25550

1 Input exposure duration here 10 Input exposure fequency here 10 55

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2763
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range
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0.0129
1700000
58.8
see below
0.14
range

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1.445152E+05

Bennet and Furtaw (2004) EST38: 2142-2152

Air concentration in an enclosed space, at equilibrium, after 7 days post carpet installation (mg/m³)

64281.046283

F x VRF)]

0.01



4809	4746	4670	4136	3618
160049.6	110951.8	80198.9	24926.7	13390.8



ADDENDUM II TO REPORT:

EXPOSURE AND SCREENING-LEVEL RISK ASSESSMENT FOR
CARPET FIBER AND FOOD WRAP SCENARIOS
ASSOCIATED WITH PIGMENT RED 144/214
APRIL 11, 2005 REVISION

STEP-BY-STEP CALCULATIONS GUIDE

Prepared for Clariant Corporation 4000 Monroe Road Charlotte, NC 28205

Prepared by BBL Sciences

November 14, 2006

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1. Introduction

On August 18, 2006, BBL Sciences submitted Addendum II to the April 11, 2005 report titled Exposure and Screening-Level Risk Assessment for Carpet Fiber and Food Wrap Scenarios Associated with Pigment Red 144/214. The objective of Addendum II was to incorporate the United States Environmental Protection Agency's (USEPA's) requested assumption of the volatilization potential and minimum air exchange rate (8.4 room air exchanges per day) of polychlorinated biphenyl (PCB) and to demonstrate calculations for a finite mass of PCB volatilizing into indoor air. On October 12, 2006, the USEPA requested a supplemental clarification of the calculations presented in Addendum II. BBL Sciences has prepared this document to clarify previously submitted calculations. Please note that the results for safe concentrations of PCBs in carpet presented here have changed from those reported in the August 18, 2006 Addendum due to the final adjustment of exposure durations (to ensure that PCB concentrations in room air are nil) and the EPA-recommended, worst-case room ventilation rate of 0.35 exchanges per hour.

2. Key Equations

The key equations included in this section have previously been presented, and their usage and accuracy has been acknowledged by the USEPA. The equations have been coded into a Microsoft Excel® spreadsheet prior to calculation. The USEPA has been supplied with a copy of this spreadsheet.

2.1 Non-Cancer Hazard

The following equation calculates a carpet fiber concentration that does not pose a potential for adverse effects. The calculation considers exposure via dermal, ingestion, and inhalation pathways.

$$CNC_{Corpet} = \frac{THQ \cdot BW \cdot AT_{rc}}{ED \cdot EF \left[\left(\frac{1}{RfD} \cdot \frac{IR \cdot BioAF}{10^6 mg/kg} \right) + \left(\frac{1}{RfD} \cdot \frac{SA \cdot AF \cdot DERM}{10^6 mg/kg} \right) + \left(\frac{1}{RfD} \cdot IHR \cdot \frac{1}{VF} \cdot RF \right) \right]}$$

Equation 1

Where:

CNC_{Curpet} represents the risk-based concentration in carpet fiber associated with hazard quotient of 1;

THO represents the target hazard quotient (unitless);

BW represents body weight (kilogram [kg]);

RfD represents the non-cancer reference dose (milligrams per kilogram body weight per day (mg/kg BW/day);

 AT_{nc} represents the non-cancer averaging time (days);

ED represents the exposure duration (years [yr]);

EF represents the exposure frequency (days/yr)l;

IR represents the dust ingestion rate (mg/day);

BioAF represents thebioavailability factor for ingestion (unitless);

SA represents the contact skin surface area (square centimeters per day [cm²/day]);

AF represents dust adherence factor (mg/cm²);

DERM represents the dermal absorption factor (unitless);

IHR represents the inhalation rate (cubic meters per day [m³/day]);

VF represents the volatilization factor (m³/kg); and

RF represents the retention factor (unitless).

The volatilization factor (VF) used in the above equation was calculated via a set of concentration relationships derived experimentally for an enclosed chamber containing a carpet sample impregnated with a substance of interest (Bennet and Furtaw, 2004, citing Won et al., 2000). The relationships describing carpet surface to air partitioning (K_{SA}) were as follows:

$$K_{SA} = \frac{\frac{k_s}{k_d}}{d_{so}} = 10^{3.82 - 0.62 \log VP}$$
 Equation 2

Where:

$$\frac{k_s}{k_d} = \frac{M}{C_s}$$
 Equation 3

Substituting Equation 3 into Equation 2 and solving for M (mass of PCB per area of carpet [mg/m²]) yields:

$$M = (d_w \cdot 10^{3.82 - 0.62 \log VP} \cdot C_\rho)$$
 Equation 4

Where:

 k_s represents the adsorption coefficient (meters per hours [m/hr]);

 k_d represents the desorption coefficient (m/hr);

 d_w represents the carpet thickness (m);

VP represents vapor pressure (Pa);

 C_g represents the acceptable concentration of PCB in air from Equation 1 and 9 (mg/m³); and

M represents the mass of PCB per area of carpet (milligrams per square meter $[mg/m^2]$).

To express M on carpet weight basis (M_{cw} ; mg/kg), this parameter can be divided by carpet face weight (FW; kg/m^2) such that:

$$M_{cw} = \frac{(d_w \cdot 10^{3.82 - 0.62 \log VP} \cdot C_g)}{FW}$$
 Equation 5

This results in a PCB concentration in mass of PCB per mass of carpet. Furthermore, under general household conditions, ventilation is provided to maintain proper air quality. Therefore, the M_{cw} term (mass of PCB per mass of carpet) must allow for an AE (unitless). This accounts for air turnover rates

in the home, without which unrealistically high PCB air concentrations might result. Thus, Equation 5 is modified to:

$$M_{cw} = \frac{d_w \cdot 10^{3.82 - 0.62 \log VP} \cdot C_g \cdot AE}{FW}$$
 Equation 6

Finally, the volatilization factor (VF; m^3/kg) was derived by dividing M_{cw} by the air concentration term C_g to yield Equation 7:

$$VF = \frac{M_{cw}}{C_g} = \frac{(d_w \cdot 10^{3.82 - 0.62 \log VP} \cdot AE)}{FW}$$
 Equation 7

The VF was inserted into Equation 1 to calculate an acceptable carpet concentration attributable to total PCB (tPCB) volatilization.

Given that C_g is calculated in Equations 1 and 9 (using the inhalation assumptions [e.g., $(THQ*BW*AT_{nc})/(ED*EF*1/RfD*IHR*RF) = C_g]$), VF was inserted in this portion of the equation to derive an acceptable concentration in carpet fiber $(M_{cw}; mg/kg)$ for the inhalation component of the overall equation:

$$VF*C_g = M_{cw}$$
 Equation 8

2.2 Cancer Risk

The following equation calculates a carpet fiber concentration that does not pose an unacceptable risk of cancer. The calculation considers exposure via dermal, ingestion, and inhalation pathways.

$$CC_{Carpet} = \frac{TR \cdot BW \cdot AT_{c}}{ED \cdot EF \left[\left(\frac{CSF \cdot IR \cdot BioAF}{10^{6} mg/kg} \right) + \left(\frac{CSF \cdot SA \cdot AF \cdot DERM}{10^{6} mg/kg} \right) + \left(\frac{CSF \cdot IHR \cdot \frac{1}{VF} \cdot RF}{10^{6} mg/kg} \right) \right]}$$
Equation 9

Where:

CC_{Carpet} represents the risk-based concentration in carpet associated with 1 x 10⁻⁶ cancer risk;

TR represents the target cancer risk;

BW represents the body weight (kg);

CSF represents the cancer slope factor (mg/kg BW/day)⁻¹;

 AT_c represents the cancer averaging time (days);

ED represents the exposure duration (yrs);

EF represents the exposure frequency (days/yr);

IR represents the dust ingestion rate (mg/day);

BioAF represents the bioavailability factor for ingestion (unitless);

SA represents the contact skin surface area (cm²/day);

AF represents the dust adherence factor (mg/cm²);

IHR represents the inhalation rate (m³/day);

DERM represents the dermal uptake factor (unitless);

VF represents the volatilization factor (m³/kg); and

RF represents the retention factor (unitless).

3. Model Parameters

Input parameters used to parameterize the above equations are summarized in Table 1. The paragraphs below discuss each input parameter in detail.

Table 1. Exposure and Risk Model Input Parameters

Parameter	Value	Source
General	<u> </u>	<u> Parantis de la lacción de la companya de la compa</u>
Exposed population: Young Children (yrs)	1 to 10	USEPA (2000)
Body weight (1 to 10 yrs old; kg)	21.8	USEPA (2000)
Carpet life span (maximum; yrs)	10	Bigger and Bigger (2004)
Exposure duration (years)	1 to 10	Calculated ¹
Exposure frequency (days/yr)	3 to 350	Calculated ¹ ; USEPA (1997, 2002)
Life expectancy (yrs)	70	USEPA (1997; 2002)
Averaging time: non-cancer (maximum; days)	365 to 3,650	Calculated ¹ ; USEPA (1997; 2002)
Averaging time: cancer (days)	25,550	USEPA (1997; 2002)
Maximum PCB carpet concentration (mg PCB/kg carpet)	14.1	Estimated; Clariant
Total PCB mass (mg) in a hypothetical room	599	Calculated
Ingestion		
Dust (soil) ingestion rate (children; mg dust/day)	55	Moya et al. (2004)
Bioavailability of PCB in fiber (%)	1, 5, 10, 50, and 100	Assumption
Inhalation	I	
Inhalation rate (1 to 10 yrs old; m³/day)	10.4	USEPA (2000)
Complete air exchange rate (1/day)	8.4	USEPA (1995)
Vapor pressure of PCB 44/70 mixture (Pascals [Pa])	0.0069	MacKay et al. (1992)
Room volume (hypothetical; m³)	50	Assumption
Floor area (hypothetical; m²)	25	Assumption
Carpet thickness (m)	0.01286	RPA (2004)
Carpet area mass (face weight; kg/m²)	1.7	Carpet USA (2004)
Room temperature (degrees Kelvin (K])	293	Assumption
Molecular weight of air (g/mol)	29	Calculated
Molecular weight of PCB (g/mol)	292	Calculated
Atmospheric pressure (atm)	1	Assumption
Molar volume of air (cm ³ /mol)	20.1	Calculated
Molar volume of PCB (cm³/mol)	268	Calculated
Diffusivity of PCB in air (m²/day)	0.416	Calculated; Fuiler et al. (1966) ²
Vapor pressure of PCB 44/70 mixture (Pa)	0.0069	MacKay et al. (1992)
Ideal gas constant (Pa x m³/mol x K)	8.314	Constant
Retention factor (unitless)	0.0001 to 1	Assumption
Dermal		
Dust adherence factor for children post-activity indoors on hands, arms, legs, and feet (mg/cm²)	0.00724	USEPA (2000)

Parameter	Value	Source
Contact skin surface area during warm-weather play with 32% skin exposed (cm²/day)	2,763	USEPA (2000)
Dermal uptake factor	0.14	USEPA (2001)
Hazard and Risk Reference Values	· · · · · · · · · · · · · · · · · · ·	¥ = 100 m
Target hazard quotient	1	USEPA (1997, 2002)
Non-cancer reference dose (mg/kg BW/day)	0.00002	USEPA (2002)
Cancer slope (mg/kg BW/day) ⁻¹	0.07	USEPA (2002)
Target cancer risk	1 x 10 ⁻⁶	USEPA (1997, 2002)
Target lifetime average daily dose (mg/kg BW/day)	0.000014	Equal to acceptable risk over cancer slope

3.1 **Body Weight**

The receptor of interest in the carpet scenario was a young child who was expected to be in direct contact with carpeted surfaces as a result of normal daily activities such as playing, walking, and crawling. The range of age within this group can conceivably span from 1 to 10 years. The calculated average body weight for children of that age was 21.8 kg (USEPA, 2000) (Table 1).

3.2 Ingestion Parameters

The primary mode of tPCB intake in this exposure scenario was assumed to be via the incidental ingestion of carpet fibers/dust as a result of the mouthing of carpet surfaces, toys, hands, and feet. Because no ingestion rate data for the carpet fiber were readily available in the published literature, a conservative assumption was made that the carpet fiber intake by children is comparable to that of soil dust. According to Moya et al. (2004), children consume an average of 193 mg of soil and dust per day. However, the authors also stated that the daily consumption of soil alone is 138 mg/day. Therefore, an average dust ingestion rate of 55 mg/day can be estimated by subtracting 138 mg/day from 193 mg/day. That value was used to approximate the daily fiber ingestion rate (Table 1). A bioavailability factor was introduced into this component of the exposure/risk model to account for the proportion of the tPCB in carpet that may be dislodged via digestive tract activities. This factor was set to range from 1% to 100% (Table 1) due to uncertainty as to its real empirical magnitude.

3.3 Inhalation Parameters

The inhalation rate of the receptor was set at 10.4 m³/day, which is the average estimate for children ranging in age from 1 to 10 years old (USEPA, 2000) (Table 1). The tPCB vapor contribution to the

¹Retention factor-dependent ²D_{Air}= 10^{-3} * $(t_{Air}^{1.75}$ * $(1/M_{Air} + 1/M_{PCB})^{0.5})/P(V_{Air}^{0.93} + V_{PCB}^{0.93})^2$

overall exposure burden was estimated via a set of empirical models derived from air chamber experiments (Equations 2 to 8; Bennet and Furtaw, 2004). The required parameters in these models include carpet thickness, carpet area mass (also called face weight), and vapor pressure. Average carpet thickness was set to 0.0129 m, and face weight was set to 1,700,000 mg/m² (1.7 kg/m²) based on information obtained from the carpet industry (RPA, 2004; Carpet USA, 2004) (Table 1). The vapor pressure parameter was set to 0.0069 Pa and consisted of a mean of all values for PCB congeners 44 and 70 reported in the compendium by MacKay et al. (1992) (Table 1). To account for dilution due to ventilation, an AE was added to Equation 6. The value of that factor was 8.4 air exchanges per day based on the minimum ventilation rate required by USEPA.

3.4 Dermal Uptake Parameters

According to the USEPA (2000), the skin surface area available for contact during warm-weather play of children, with 32% of the total skin surface area exposed, is 2,763 cm²/day (Table 1). The adherence factor, or the amount of material remaining on the skin after contact, was estimated at 0.00724 mg/cm² (USEPA, 2000). This value reflects soil adherence for children: post-activity; indoors; and on hands, arms, legs, and feet. An assumption was made that carpet fibers behave similarly to soil particles. The USEPA's default value for the dermal absorption factor for tPCB in soil of 14% (USEPA, 2001) was adopted as the default value in this screening-level risk assessment.

3.5 Hazard and Risk Reference Values

The non-cancer reference dose for PCB was 0.00002 mg/kg/day (reference dose for Aroclor 1254; USEPA, 2002). The cancer slope factor was 0.07 (mg/kg/day)⁻¹ and represented the lowest risk and persistence category recommended by the USEPA (2002). The target risk used in the calculation was the low end of the USEPA's "acceptable risk range" of 1 in 1 million exposed individuals (1 x 10⁻⁶) (USEPA, 1996, 1997, 2000) (Table 1). The target hazard quotient was set to 1.

3.6 Temporal Parameters

The time scale of the exposure and risk estimate was set to coincide with the useful life span of a residential carpet. According to an industry source, carpet warranties may span from 5 to 20 years. However, a typical carpet lasts approximately 10 years (Bigger and Bigger, 2004). Therefore, the maximum exposure duration in this assessment was assumed to be 10 years. For the cancer risk assessment, a default life expectancy of 70 years was used as the averaging time in the derivation of the lifetime average daily dose (25,550 days) (USEPA 1997, 2002) (Table 1).

Note that the retention factor (RF) was set to vary from 0.0001 to 1, depending on the exposure scenario. Therefore, the range of time needed for PCB to volatilize from the carpet varies accordingly, and this directly affects the estimates of exposure frequencies and duration in each scenario. To simulate this, the exposure frequency was set to vary for each RF scenario as the finite mass of PCB volatilizes from carpet at a RF-dependent rate (Table 1). However, consistent with default assumptions, the exposure frequency did not exceed 350 days per year (at the event frequency of one event per day; USEPA, 1997, 2002) and the exposure duration of 10 years.

The method to estimate the times of total exhaustion of PCB from carpet via volatilization and subsequent clearance from a hypothetical room (at the lowest recommended room ventilation rate [i.e. 8.4 air exchanges/day]) for each RF was based on the flux-based approach of Bennett and Furtaw (2004) for indoor residential fate modeling of pesticides on carpet. This methodology is described below.

3.6.1 PCB Mass Transfer Rate

The flux-based transfer of PCB from carpet into air was presented and used by BBL Sciences in previous assessments of PCB volatilization. Its accuracy was acknowledged by the USEEPA in its October 12, 2006 email correspondence.

The mass-transfer rate (MTR) algorithm is as follows:

$$MTR_{PCB} = SA_{Carpet} \times \frac{D_{Air}}{T_{Carpet}} \left(\frac{VP_{PCB}}{R_C \times t_{Air}} \right)$$
 Equation 10

Where:

 MTR_{PCB} represents the mass transfer rate (mol PCB/room-day); SA_{Carpet} represents the carpet surface area (m²); D_{Altr} represents the diffusivity of PCB in air (m²/day); T_{Carpet} represents the carpet thickness (m); VP_{PCB} represents a vapor pressure of PCB 44/70 mixture (Pa); Rc represents ideal gas constant (Pa x m³/mol x K); and

 t_{Air} represents ambient air temperature (K).

 MTR_{PCB} is converted to a mg basis by dividing the product of Equation 10 by the molecular weight of PCB (292,000 mg/mol). It is also assumed that the MTR_{PCB} is directly proportional to the RF (i.e., as the RF decreses, the MTR_{PCB} decreases proportionally; see Table 2).

The maximum flux rates estimated by Equation 10 for each RF (and MTR_{PCB}) are presented below (Table 2). Given that the total mass of PCB in a hypothetical room (25 m²) is finite at 599 mg PCB (i.e., 14.1 mg PCB/kg x 1.7 kg carpet/m² x 25 m²), the amount of time needed for complete volatilization will vary according to the flux rate (i.e. volatilization time = the total mass of PCB in a hypothetical room divided by the flux rate). For example, for the retention factor scenario of 1 (where MTR_{PCB} is 668 mg PCB per room per day), complete volatilization will take 0.89 days (i.e., 599 mg PCB per room divided by 668 mg PCB per room per day yields 0.89 days). Because there will be some lag between the point in time when the last of the PCB volatilizes into air (t_{final}; 0.89 days in the example) and the point in time when the air concentration in a room reaches near zero (to) (due to ventilation; parts per quadrillion [ppq] range), we extended the potential duration to airborne PCB by several days (based on air concentration calculations at ventilation rate of 8.4 exchanges/day). In other words, we accounted for the dilution (room ventilation) of residual PCB in ambient air after the carpet source was completely exhausted. The methodology was to keep dividing the room concentration at t_{final} (approximately 1.43 mg/m³ [i.e., 599 mg PCB divided by the room volume of 50 m³ divided by the ventilation rate of 8.4 exchanges per day for Day 1]) by the ventilation rate of 8.4 exchanges per day until the air concentration reached ppq range. For this example, the total time for the room to clear will be approximately 10 days. According to MTR_{PCB} calculations, as much as 668 mg PCB could have evaporated into the ambient air on Day 1. However, only 599 mg PCB was available for that process. Therefore, we use 599 mg PCB in our calculations.

For RF=0.01, the time to complete volatilization was much longer. It was estimated at 89.7 days (i.e. 599 mg PCB per room divided by 6.68 mg PCB per room per day yields 89.7 days). To calculate the ventilation time until the room air concentration reaches near zero (Table 2), we divided the steady-state air concentration of 0.018059 mg/m³ (the air concentration when the carpet PCB becomes exhausted on day 90) eight times by the ventilation rate of 8.4 exchanges/day. Therefore, the total time when PCB is present in air will be 98 days (this number was rounded off to 100 for the purpose of running the calculations).

The final times to complete volatilization are included in Table 2. These estimates formed the basis for exposure frequencies and exposure durations used in the exposure scenarios. Please note that exposure frequencies (EFs) were rounded up or set at default maximum values, if high enough (i.e., in the case of RF, 0.001 and 0.0001). The exposure durations (EDs) were set either to 1 year if the

volatilization times were short, the year equivalent (i.e., 894 days/ 365 days = 2.45 years), or a maximum of 10 years (the life of the carpet) for RF of 0.0001. Therefore, the EFs and EDs for a given RF were as follows.

Table 2. Parameters Used to Derive Exposure Frequencies and Durations for Each Retention Factor

RF	Flux Rate (mg-room/day)	Volatilization Time (days)	Ventilation Time (days)	EF (days/year)	ED (years)
1.0	668	0.897	10	10	1
0.01	6.68	89.7	8	100	1
0.005	3.34	179	7	180	1
0.001	0.668	897	6	350	2.45
0.0001	0.0668	8,967	4	350	10

The usage of these parameters was as follows. To develop a range of risk-based concentrations in carpet for non-cancer and cancer hazard/risk at given bioavailability and RFs, Equations 1 and 9 were populated with Table 1 constants as well as Table 2 variables so that every possible combination of constants and variables was satisfied. Table 3 lists the combinations of variables used. Table 4 lists the results for acceptable concentrations in carpet fiber.

Table 3. Calculations Matrix Used to Derive Acceptable Concentrations in Carpet Fiber

Oral Bioavailability	Retention Factor							
Factor	0.0001	0.001	0.005	0.01	1			
Non-Cancer Hazard								
	EF=350	EF=350	EF=180	EF=100	EF≂10			
0.01	ED=10	ED=2.47	ED=1	ED=1	ED=1			
	AT=3,650	AT=902	AT=365	AT=365	AT=365			
	EF=350	EF=350	EF=180	EF=100	EF=10			
0.05	ED=10	ED=2.47	ED=1	ED=1	ED=1			
	AT≃3,650	AT=902	AT=365	AT=365	AT=365			
	EF=350	EF=350	EF=180	EF=100	EF=10			
0.10	ED=10	ED=2.47	ED=1	ED=1	ED≃1			
	AT=3,650	AT=902	AT=365	AT=365	AT=365			
	EF=350	EF=350	EF=180	EF=100	EF=10			
0.50	ED=10	ED=2.47	ED≂1	ED≂1	ED=1			
	AT=3,650	AT=902	AT=365	AT=365	AT=365			
	EF=350	EF=350	EF=180	EF=100	EF=10			
1.00	ED=10	ED=2.47	ED=1	ED=1	ED=1			
	AT=3,650	AT=902	AT=365	AT=365	AT=365			
Cancer Risk								
	EF=350	EF=350	EF=180	EF=100	EF=10			
0.01	ED=10	ED=2.47	ED=1	ED=1	ED=1			
	AT=25,550	AT=25,550	AT=25,550	AT=25,550	AT=25,550			
	EF=350	EF=350	EF=180	EF=100	EF=10			
0.05	ED=10	ED=2.47	ED≃1	ED≔1	ED=1			
	AT=25,550	AT=25,550	AT=25,550	AT=25,550	AT=25,550			
	EF=350	EF=350	EF=180	EF=100	EF=10			
0.10	ED=10	ED=2.47	ED=1	ED=1	ED≂1			
	AT=25,550	AT=25,550	AT=25,550	AT=25,550	AT=25,550			
	EF=350	EF=350	EF=180	EF=100	EF=10			
0.50	ED=10	ED=2.47	ED=1	ED=1	ED=1 :			
	AT=25,550	AT=25,550	AT=25,550	AT=25,550	AT=25,550			
	EF=350	EF=350	EF=180	EF=100	EF=10			
1.00	ED=10	ED=2.47	ED=1	ED=1	ED=1			
N	AT=25,550	AT=25,550	AT=25,550	AT=25,550	AT=25,550			

Note:

EF=exposure frequency (days/year); ED=exposure duration (years); AT=averaging time (days)

Table 4. October 2006 Revised Risk-Based Concentrations (mg/kg) of tPCB in Carpet Fiber for Child Non-Cancer and Cancer Risk Scenarios, Assuming Complete Volatilization from Carpet Surface and Finite PCB Mass

Oral	Acceptable Concentration in Carpet Fiber (mg tPCB/kg)								
Bioavailability	Retention Factor								
Factor	0.0001	0.001	0.005	0.01	1				
Non-Cancer Hazard	i		1						
0.01	135	129	212	320	96.2				
0.05	81.7	79.6	139	222	94.9				
0.10	54.7	53.7	97.0	160	93.4				
0.50	15.0	14.9	28.4	49.9	82.7				
1.00	7.86ª	7.84ª	15.1	26.8	72.4				
Cancer Risk				<u> </u>	^				
0.01	675	2,620	10,624	16,005	4,809				
0.05	408	1,611	6,949	11,095	4,746				
0.10	273	1,088	4,852	8,020	4,670				
0.50	75.0	302	1,421	2,493	4,136				
1.00	39.3	159	754	1,339	3,618				

Note:

^aThe result for an oral bioavailability factor of 0.53 is 14.2 mg/kg.

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